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Application of a modified FFT to product type integration

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Abstract

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An automatic integration scheme is proposed for evaluating the so-called product type (indefinite) integral $Q(K, f)=\int_x^y K(t)f(t)\,dt$, $-1 \leqslant x, y \leqslant 1$, where $f(t)$ is assumed to be a smooth function and $K(t)$ are some singular or badly-behaved functions. Typical examples for $K(t)$ are $\ln|t-c|$, $|t-c|^{\alpha}$, $\alpha > -1$, Cauchy principal value $1/(t-c)$ and $e^{i\omega t}$, $|\omega| \gg 1$. The function $f(t)$ is approximated by a truncated Chebyshev series $p_N(t)$ of degree N, whose coefficients are efficiently computed using the FFT. The approximation $Q_N(K, f)$ to the integral $Q(K, f)$ is given by $Q(K, p_N)$. The sequence $\{p_N(t)\}$ is recursively generated until the required tolerance for the integral is satisfied. To enhance the efficiency of the automatic quadrature, the degree N is increased more slowly than doubling, which is usually the case. The evaluations of $Q_N(K, f)=Q(K, p_N)$ for a set of $\{(x, y, c)\}$ can be efficiently made by using recurrence relations for the singular kernels $K(t)$ above. Numerical examples for the algebraic singular kernel $K(t)=|t-c|^{\alpha}$, $\alpha > -1$, are included.

Keywords: Automatic quadrature, product integral, singular integral, indefinite integral, Chebyshev polynomial, FFT, recurrence relation.

1. Introduction

We describe an automatic quadrature method for the so-called product type (indefinite) integral

$$Q(K, f)=\int_x^y K(t;\, c)f(t)\,dt, \quad -1 \leqslant x, y \leqslant 1, \tag{1}$$

where $f(t)$ is assumed to be a smooth function and $K(t;\, c)$ is a badly-behaved or singular function such as $|t-c|^{\alpha}$, $\alpha > -1$, $\ln|t-c|$, $-1 \leqslant c \leqslant 1$, Cauchy principal value $1/(t-c)$,

$-1 < c < 1$, or e^{ict}, $|c| \gg 1$. There seems to exist very little literature on the numerical evaluation of the indefinite integral (1), while there are many investigations [3,5,16–19] into the definite integral

$$I(K, f) = \int_{-1}^{1} K(t;\ c) f(t)\, dt. \tag{2}$$

The present scheme is an extension of the Clenshaw and Curtis quadrature method (henceforth abbreviated to CC method) [2] to the integral (1). In the CC method, the function $f(t)$ is approximated by a sum of the Chebyshev polynomials $T_k(t)$ of the first kind:

$$p_N(t) = \sum_{k=0}^{N}{}'' a_k^N T_k(t), \quad -1 \leqslant t \leqslant 1. \tag{3}$$

The double prime denotes the summation where the first and last terms are halved. The coefficients a_k^N are determined so that $p_N(t)$ interpolates $f(t)$ at the abscissae $t_j^N = \cos(\pi j/N)$, $0 \leqslant j \leqslant N$, which are the zeros of the polynomial $\omega_{N+1}(t)$ defined by

$$\omega_{N+1}(t) = T_{N+1}(t) - T_{N-1}(t) = 2(t^2 - 1)U_{N-1}(t), \tag{4}$$

where $U_k(t)$ is the Chebyshev polynomial of the second kind defined by $U_k(t) = \sin(k+1)\theta/\sin\theta$, $t = \cos\theta$. If $f(t)$ is a smooth function, the truncated Chebyshev series (3) converges rapidly.

In their adaptive quadrature programs [16], Piessens et al. used the approximation $I_N(K, f)$ below to the definite integral $I(K, f)$ (2):

$$I_N(K, f) = I(K, p_N) = \sum_{k=0}^{N}{}'' a_k^N\ I(K, T_k), \tag{5}$$

where the so-called modified moments $I(K, T_k)$ can be evaluated for some useful kernel functions K by means of recurrence relations. If $K(t;\ c) = 1$ in (2), the quadrature scheme $I_N(1, f)$ (5) reduces to the CC method.

In this paper, to make an automatic quadrature rule of nonadaptive type for the indefinite integral (1) with smooth function $f(t)$, we extend the scheme (5) and obtain an approximation $Q_N(K, f)$:

$$Q_N(K, f) = \int_{x}^{y} K(t;\ c) p_N(t)\, dt = Q(K, p_N). \tag{6}$$

Section 2 shows that the evaluation of $Q(K, p_N)$ (6) with $-1 \leqslant x, y \leqslant 1$, can be efficiently made by using the three-term recurrence relations depending on the value of c, but not depending on x and y for the kernels $K(t;\ c)$ mentioned above.

It is well known that the Fast Fourier Transform (FFT) is useful for computing the coefficients $\{a_k^N\}$ in (3); see (33) and [1,8], where by doubling N the computation can be repeated, reusing the previous values until an error criterion is satisfied. It is advantageous to have more chances of checking the stopping criterion than doubling of N for enhancing the efficiency of automatic quadrature. In [13] we described the recursive method to generate the sequence of the interpolating polynomials $\{p_N(t)\}$ by increasing N as follows:

$$N = 3 \times 2^n, 4 \times 2^n, 5 \times 2^n, \quad n = 1, 2, 3, \ldots, \tag{7}$$

and by using the FFT. In Section 3 we briefly review this iterative scheme based on the FFT. Section 4 discusses error estimates for the approximate integral (6). Numerical results for the case $K(t;\ c)=|t-c|^{\alpha}$, $\alpha>-1$, are given in Section 5.

2. Recurrence relations

We will derive the recurrence relations for evaluating the approximation (6) with each kernel function $K(t;\ c)$ through the first-order differential equations.

2.1. Oscillatory kernel

Now we show that for a polynomial $p_N(t)$ of degree N, we can use an auxiliary polynomial $F_N(t)$ of degree N to write the approximation $\int_x^y \mathrm{e}^{\mathrm{i}ct}\, p_N(t)\,\mathrm{d}t$ to the oscillatory integral $\int_x^y \mathrm{e}^{\mathrm{i}ct}\, f(t)\,\mathrm{d}t$ as follows:

$$\int_x^y \mathrm{e}^{\mathrm{i}ct} p_N(t)\,\mathrm{d}t=\frac{\mathrm{e}^{\mathrm{i}cy}F_N(y)-\mathrm{e}^{\mathrm{i}cx}F_N(x)}{\mathrm{i}c}. \tag{8}$$

Differentiating both sides of (8) with respect to y (or x), and taking y again as variable t, we obtain the first-order differential equation

$$\frac{F_N'(t)}{\mathrm{i}c}+F_N(t)=p_N(t), \tag{9}$$

which is integrated to yield

$$\frac{F_N(y)-F_N(x)}{\mathrm{i}c}+\int_x^y F_N(t)\,\mathrm{d}t=\int_x^y p_N(t)\,\mathrm{d}t. \tag{10}$$

We can see that relations (8) and (9) (or (10)) are satisfied if $F_N(t)$ is chosen to be a polynomial of degree N.

To solve (10), we expand $F_N(t)$ in terms of the Chebyshev polynomials:

$$F_N(t)=\sum_{k=0}^{N}{}' b_k T_k(t), \tag{11}$$

where the prime denotes the summation whose first term is halved. Substitute (3) and (11) in (10) and use the relation

$$2\int T_k(t)\,\mathrm{d}t=\frac{T_{k+1}(t)}{k+1}-\frac{T_{k-1}(t)}{k-1}+\text{const.},\quad k\geqslant 2; \tag{12}$$

then, comparing the coefficients of Chebyshev polynomials, we have

$$b_{k-1}+\frac{2k}{\mathrm{i}c}b_k-b_{k+1}=a_{k-1}^N-a_{k+1}^N. \tag{13}$$

For convenience, we set $a_k^N=0$, $k>N$, and take $\frac{1}{2}a_N^N$ instead of a_N^N. We have omitted the dependency of the coefficients b_k in (11) on c as well as the coefficients $\{a_k^N\}$ of $p_N(t)$.

Forward and backward recursions are numerically unstable for the three-term recurrence relation (13). To eliminate this instability, we have to solve a system of linear equations [9,15] with normalizing condition

$$\sum_{k=0}^{N/2-1} \frac{b_{2k+1}}{\mathrm{i}c} + \sum_{k=0}^{N/2}{}' \frac{b_{2k}}{1-4k^2} = \sum_{k=0}^{N/2}{}' \frac{a_{2k}^N}{1-4k^2},$$

which is derived by using (11) in (10) where we set $x = -1$ and $y = 1$. Here and henceforth we conveniently assume that N is even.

2.2. Algebraic singularity

For a positive integer m, it is easily verified that a product of polynomial $(t-c)^{m-1}$ and algebraic singular kernel $K(t;\, c) = |t-c|^\alpha$ is integrated as follows:

$$\int (t-c)^{m-1} |t-c|^\alpha \,\mathrm{d}t = \frac{(t-c)^m |t-c|^\alpha}{m+\alpha} + \text{const.}, \quad \alpha > -1. \tag{14}$$

Equation (14) would indicate that we may make use of a polynomial $F_N(t)$ to write an integral including a polynomial $p_N(t)$ of degree N in the form

$$\int |t-c|^\alpha \{ p_N(t) - p_N(c) \} \,\mathrm{d}t = (t-c)|t-c|^\alpha \{ F_N(t) - F_N(c) \} + \text{const.} \tag{15}$$

Consequently, we have an expression for the integral having algebraic singular kernel $K(t;\, c) = |t-c|^\alpha$:

$$\int_x^y |t-c|^\alpha p_N(t) \,\mathrm{d}t = (y-c)|y-c|^\alpha \left\{ F_N(y) - F_N(c) + \frac{p_N(c)}{\alpha+1} \right\} - (x-c)|x-c|^\alpha \left\{ F_N(x) - F_N(c) + \frac{p_N(c)}{\alpha+1} \right\}. \tag{16}$$

Differentiating both sides of (15) gives a differential equation for $F_N(t)$:

$$(t-c)F_N'(t) + (\alpha+1)\{ F_N(t) - F_N(c) \} = p_N(t) - p_N(c). \tag{17}$$

We can see that the equation (17) is satisfied if $F_N(t)$ is chosen to be a polynomial of degree N.

Now, we solve the equation (17). Let

$$F_N'(t) = \sum_{k=0}^{N-1}{}' b_k T_k(t);$$

then it follows that

$$(t-c)F_N'(t) = \sum_{k=0}^{N} (b_{k+1} - 2cb_k + b_{k-1}) T_k(t), \tag{18}$$

$$F_N(t) - F_N(c) = \sum_{k=1}^{N} \frac{b_{k-1} - b_{k+1}}{2k} \{ T_k(t) - T_k(c) \}, \tag{19}$$

where for convenience, we set $b_N = b_{N+1} = 0$ and $b_{-1} = b_1$. In deriving (18) and (19) we have used (12) and the following relation:

$$2tT_k(t) = T_{k+1}(t) + T_{k-1}(t), \quad k \geqslant 1. \tag{20}$$

Substituting (3), (18) and (19) into (17) and comparing both sides, we have a recurrence relation

$$\left(1-\frac{\alpha+1}{k}\right)b_{k+1}-2cb_k+\left(1+\frac{\alpha+1}{k}\right)b_{k-1}=2a_k^N, \tag{21}$$

where we take $\frac{1}{2}a_N^N$ instead of a_N^N. The backward recursion of (21) is numerically stable for $-1 \leqslant c \leqslant 1$ with the starting values $b_N = b_{N+1} = 0$.

By using the same polynomial as $F_N(t)$ obtained above, we have for $K(t;\ c) = |t-c|^\alpha \operatorname{sign}(t-c)$, $\alpha > -1$,

$$\begin{aligned}\int_x^y |t-c|^\alpha \operatorname{sign}(t-c)\ p_N(t)\ \mathrm{d}t &= |y-c|^{\alpha+1}\left\{F_N(y)-F_N(c)+\frac{p_N(c)}{\alpha+1}\right\}\\ &\quad -|x-c|^{\alpha+1}\left\{F_N(x)-F_N(c)+\frac{p_N(c)}{\alpha+1}\right\}.\end{aligned} \tag{22}$$

2.3. Logarithmic kernel

Let m be a positive integer. Then we can see that

$$\int (t-c)^{m-1} \ln|t-c|\ \mathrm{d}t = (t-c)^m \frac{\ln|t-c|-1/m}{m} + \text{const.},$$

which would suggest that we may use two polynomials $G_{N+1}(t)$ and $H_{N+1}(t)$ of degree $N+1$ to express an indefinite integral of a polynomial $p_N(t)$ of degree N and kernel $K(t;\ c) = \ln|t-c|$ as follows [10]:

$$\int \ln|t-c|\ p_N(t)\ \mathrm{d}t = \{G_{N+1}(t) - G_{N+1}(c)\} \ln|t-c| - H_{N+1}(t) + \text{const.} \tag{23}$$

In fact, differentiating both sides of (23) yields

$$\ln|t-c|\ p_N(t) = \frac{G_{N+1}(t)-G_{N+1}(c)}{t-c} + G'_{N+1}(t)\ln|t-c| - H'_{N+1}(t). \tag{24}$$

It is possible to have $G_{N+1}(t)$ and $H_{N+1}(t)$, two polynomials of degree $N+1$ satisfying (24) if they are chosen to satisfy the differential equations

$$G'_{N+1}(t) = p_N(t), \tag{25}$$

$$H'_{N+1}(t) = \frac{G_{N+1}(t)-G_{N+1}(c)}{t-c}. \tag{26}$$

Now, to solve (25) and (26) let us write

$$G_{N+1}(t) - G_{N+1}(c) = (t-c)\sum_{k=0}^{N}{}' b_k T_k(t), \tag{27}$$

then from (12) and (26) we have, except for a constant,

$$H_{N+1}(t) = \sum_{k=1}^{N+1} \frac{b_{k-1}-b_{k+1}}{2k} T_k(t). \tag{28}$$

On the other hand, from (3), (12) and (25) we obtain

$$G_{N+1}(t) - G_{N+1}(c) = \sum_{k=1}^{N+1} \frac{a_{k-1}^N - b_{k+1}^N}{2k} \{T_k(t) - T_k(c)\}. \tag{29}$$

Comparing (27) and (29) and using (20) gives

$$b_{k+1} - 2cb_k + b_{k-1} = \frac{a_{k-1}^N - a_{k+1}^N}{k}, \tag{30}$$

where we take $\frac{1}{2}a_N^N$ instead of a_N^N. The backward recursion of (30) is numerically stable with the starting values $b_{N+1} = b_{N+2} = 0$ if $-1 \leqslant c \leqslant 1$.

2.4. Cauchy principal value integral

For the approximation (6) to the Cauchy principal value integral with $K(t;\, c) = 1/(t-c)$, $-1 < c < 1$, one can write

$$\mathrm{P}\int_x^y \frac{p_N(t)}{t-c}\,\mathrm{d}t = \int_x^y \frac{p_N(t) - p_N(c)}{t-c}\,\mathrm{d}t + p_N(c)\,\mathrm{P}\int_x^y \frac{1}{t-c}\,\mathrm{d}t. \tag{31}$$

Now, we can expand the integrand in the first term of the right-hand side of (31) in the form

$$\sum_{k=0}^{N-1} b_k T_k(t).$$

If we note the relation (20), the coefficients $\{b_k\}$ are seen to satisfy the recurrence relation

$$b_{k+1} - 2cb_k + b_{k-1} = 2a_k^N, \tag{32}$$

and are stably computed in the backward direction with the starting values $b_N = b_{N+1} = 0$ where we take $\frac{1}{2}a_N^N$ instead of a_N^N.

3. Chebyshev coefficients and the FFT

We will briefly review the iterative procedure for computing the sequence $\{p_N(t)\}$ (3) of the truncated Chebyshev series by increasing N as in (7) and by using the FFT for real data. For details, see [13].

We begin with the sample points for $p_N(t)$ to interpolate $f(t)$. We proposed in [12,13] a sequence of uniform distribution $\{\beta_j\}$ which is a modification of the van der Corput sequence [6] and satisfies the recurrence relation

$$\beta_{2j} = \tfrac{1}{2}\beta_j, \quad \beta_{2j+1} = \beta_{2j} + \tfrac{1}{2}, \qquad j = 1, 2, \ldots,$$

with the starting value $\beta_1 = \frac{3}{4}$. The set of the abscissae $\{\cos 2\pi\beta_j\}$, $j = -1, 0, 1, \ldots$, where we put $\beta_{-1} = 0$ and $\beta_0 = \frac{1}{2}$, is a sequence of Chebyshev distribution [14], which makes the sequence of interpolating polynomials converge uniformly on $[-1, 1]$ for functions analytic on $[-1, 1]$. The polynomial $p_N(t)$ interpolates $f(t)$ at the first $N+1$ points of the sequence $\{\cos 2\pi\beta_j\}$.

Let $N = 2^n$, $n = 2, 3, \ldots$; then the set of the $N+1$ abscissae $\{\cos 2\pi\beta_j\}$, $-1 \leqslant j < N$, agrees with $\{\cos \pi j/N\}$, $0 \leqslant j \leqslant N$, used in the CC method, that is the zeros of $\omega_{N+1}(t)$ (4). The interpolation condition $p_N(\cos \pi j/N) = f(\cos \pi j/N)$, $0 \leqslant j \leqslant N$, determines the coefficients a_k^N for $p_N(t)$ (3) as follows:

$$a_k^N = \frac{2}{N} \sum_{j=0}^{N}{}'' f\left(\cos \frac{\pi j}{N}\right) \cos \frac{\pi k j}{N}, \quad 0 \leqslant k \leqslant N. \tag{33}$$

The right-hand side of (33) is known to be efficiently computed by means of the FFT for real data [8].

We represent the polynomial $p_{5N/4}(t)$ and $p_{3N/2}(t)$ interpolating $f(t)$ at the first $\frac{5}{4}N+1$ and $\frac{3}{2}N+1$ of the abscissae $\{\cos 2\pi\beta_j\}$, respectively, in the form

$$\begin{aligned} p_{N+N/\sigma}(t) - p_N(t) &= -\omega_{N+1}(t) \sum_{k=1}^{N/\sigma} B_k^\sigma U_{k-1}(t) \\ &= \sum_{k=1}^{N/\sigma} B_k^\sigma \{T_{N-k}(t) - T_{N+k}(t)\}, \quad \sigma = 2, 4, \end{aligned} \tag{34}$$

where we have omitted the dependency of B_k^σ on N. Then , the coefficients $\{B_k^\sigma\}$ are determined to satisfy the conditions

$$p_{N+N/\sigma}(t_j^\sigma) = f(t_j^\sigma), \quad 0 \leqslant j < \frac{N}{\sigma}, \quad \sigma = 2, 4,$$

where the sample points t_j^σ are defined by

$$t_j^\sigma = \cos \frac{2\pi\sigma(j+\beta_\sigma)}{N} \quad \text{or} \quad T_{N/\sigma}(t_j^\sigma) - \cos 2\pi\beta_\sigma = 0. \tag{35}$$

This is because the set of the additional N/σ abscissae $\{\cos 2\pi\beta_j\}$, $N \leqslant j < N/\sigma$, for $p_{N+N/\sigma}(t)$ coincides with $\{t_j^\sigma\}$ [13]. If the set of $\frac{1}{2}N$ sample points $\{\cos 4\pi(j+\beta_3)/N\}$, $0 \leqslant j < \frac{1}{2}N$, which coincides with $\{\cos 2\pi\beta_j\}$, $\frac{3}{2}N \leqslant j < 2N$, is added to the set of abscissae for $p_{3N/2}(t)$, we have $2N+1$ abscissae $\{\cos \pi j/(2N)\}$, $0 \leqslant j \leqslant 2N$, for $p_{2N}(t)$. Thus the sequence of the interpolating polynomials $\{p_{3m}, p_{4m}, p_{5m}, \ldots\}$, $m = 2^n$, $n = 1, 2, \ldots$, is recursively generated. The FFT [13] is also useful for efficiently computing the coefficients $\{B_k^\sigma\}$.

4. Error estimates

Let ϵ_ρ denote the ellipse in the complex plane $z = x + \mathrm{i}y$ with foci $(-1, 0)$, $(1, 0)$ and semimajor axis $a = \frac{1}{2}(\rho + \rho^{-1})$ and semiminor axis $b = \frac{1}{2}(\rho - \rho^{-1})$ for a constant $\rho > 1$. Assume that $N = 2^n$, $n = 2, 3, \ldots$, and that $f(z)$ is single-valued and analytic inside and on ϵ_ρ. Then, the error of the interpolating polynomials $p_N(t)$ and $p_{N+N/\sigma}(t)$, where $\sigma = 2, 4$, can be expressed in terms of the contour integral [4,11], which is also expanded in the Chebyshev series [12]:

$$f(t) - p_N(t) = \frac{1}{2\pi\mathrm{i}} \oint_{\epsilon_\rho} \frac{\omega_{N+1}(t) f(z)\, \mathrm{d}z}{(z-t)\omega_{N+1}(z)} = \omega_{N+1}(t) \sum_{k=0}^{\infty}{}' V_k^N(f) T_k(t), \tag{36}$$

$$f(t) - p_{N+N/\sigma}(t) = \frac{1}{2\pi\mathrm{i}} \oint_{\epsilon_\rho} \frac{\omega_{N+1}(t)\{T_{N/\sigma}(t) - \cos 2\pi\beta_\sigma\} f(z)\,\mathrm{d}z}{(z-t)\,\omega_{N+1}(z)\{T_{N/\sigma}(z) - \cos 2\pi\beta_\sigma\}}$$
$$= \omega_{N+1}(t)\{T_{N/\sigma}(t) - \cos 2\pi\beta_\sigma\} \times \sum_{k=0}^{\infty}{}' V_k^{N+N/\sigma}(f) T_k(t), \quad \sigma = 2, 4, \tag{37}$$

respectively. In (36) and (37) the coefficients $V_k^N(f)$ and $V_k^{N+N/\sigma}(f)$ are given by

$$V_k^N(f) = \frac{1}{\pi^2 \mathrm{i}} \oint_{\epsilon_\rho} \frac{\tilde{U}_k(z) f(z)\,\mathrm{d}z}{\omega_{N+1}(z)}, \quad k \geqslant 0, \tag{38}$$

$$V_k^{N+N/\sigma}(f) = \frac{1}{\pi^2 \mathrm{i}} \oint_{\epsilon_\rho} \frac{\tilde{U}_k(z) f(z)\,\mathrm{d}z}{\omega_{N+1}(z)\{T_{N/\sigma}(z) - \cos 2\pi\beta_\sigma\}}, \quad k \geqslant 0, \ \sigma = 2, 4, \tag{39}$$

respectively. The Chebyshev function of the second kind $\tilde{U}_k(z)$ is defined by

$$\tilde{U}_k(z) = \int_{-1}^{1} \frac{T_k(t)\,\mathrm{d}t}{(z-t)\sqrt{1-t^2}} = \frac{\pi}{\sqrt{z^2-1}\,w^k} = \frac{2\pi}{(w - w^{-1})w^k}, \tag{40}$$

where $w = z + \sqrt{z^2-1}$ and $|w| > 1$ for $z \notin [-1, 1]$ [7,12].

Using (36) in (1) and (6) yields the error for the approximate integral $Q_N(K, f)$:

$$Q(K, f) - Q_N(K, f) = Q(K, f - p_N) = \sum_{k=0}^{\infty}{}' V_k^N(f) \Omega_k^N(K), \tag{41}$$

where $\Omega_k^N(K)$ is defined by

$$\Omega_k^N(K) = \int_x^y K(t;\ c)\,\omega_{N+1}(t) T_k(t)\,\mathrm{d}t, \tag{42}$$

and we have omitted the dependence of $\Omega_k^N(K)$ on x and y. Similarly, we have the error for $Q_{N+N/\sigma}(K, f)$ depending on the interpolating polynomial $p_{N+N/\sigma}(t)$ (34):

$$Q(K, f) - Q_{N+N/\sigma}(K, f) = Q(K, f - p_{N+N/\sigma})$$
$$= \sum_{k=0}^{\infty}{}' \left(\Omega_k^{N+N/\sigma}(K) + \Omega_k^{N-N/\sigma}(K) - 2\cos 2\pi\beta_\sigma\, \Omega_k^N(K)\right) \times \tfrac{1}{2} V_k^{N+N/\sigma}(f). \tag{43}$$

For $K(t;\ c) = \ln|t-c|$, $|t-c|^\alpha$ and $\mathrm{e}^{\mathrm{i}ct}$ except for $1/(t-c)$, $\Omega_k^N(K)$ can be bounded by $\Omega(K)$ independently of N, k and c as follows:

$$|\Omega_k^N(K)| \leqslant 2\left|\int_x^y |K(t;\ c)|\,\mathrm{d}t\right| \equiv \Omega(K). \tag{44}$$

Specifically, we have

$$\Omega(K)=\frac{2(|y-c|^{\alpha}(y-c)-|x-c|^{\alpha}(x-c))}{\alpha+1}$$
$$\leqslant\frac{\max(4,2^{\alpha+2})}{\alpha+1}\qquad \text{for } K=|t-c|^{\alpha}, \tag{45}$$
$$\Omega(K)\leqslant 2|y-x|\leqslant 4\qquad \text{for } K=e^{ict}, \tag{46}$$
$$\Omega(K)\leqslant 2|y-x|\left(1-\ln\left|\tfrac{1}{2}(y-x)\right|\right)\leqslant 4\quad \text{for } K=\ln|t-c|. \tag{47}$$

For the Cauchy principal value integral we have to modify the quadrature rule (6) if we wish to have the error bounded independently of the singular point c [11]. Assume that we approximate the integral $Q(K, f)$ (1) with $K(t;\, c)=1/(t-c)$ by

$$Q_N(K, f)\equiv Q(K, p_N)+\{f(c)-p_N(c)\}Q(K, 1), \tag{48}$$

where we can obtain similar expressions for $p_{5N/4}(t)$ and $p_{3N/2}(t)$ instead of $p_N(t)$. Then we have the error

$$Q(K, f)-Q_N(K, f)=Q(K, f-p_N)-\{f(c)-p_N(c)\}Q(K, 1)$$
$$=\sum_{k=0}^{\infty\,\prime} V_k^N(f)\tilde{\Omega}_k^N, \tag{49}$$

where $\tilde{\Omega}_k^N$ is defined by

$$\tilde{\Omega}_k^N=\int_x^y\frac{\omega_{N+1}(t)T_k(t)-\omega_{N+1}(c)T_k(c)}{t-c}\,\mathrm{d}t,$$

and $|\tilde{\Omega}_k^N|\leqslant 8$ when $x=-1$ and $y=1$, see [11]. It is an open problem to evaluate the bound of $|\tilde{\Omega}_k^N|$ for arbitrary values of x and y satisfying $-1<x, y<1$.

Suppose that $f(z)$ is a meromorphic function which has M simple poles at the points z_m, $m=1, 2,\ldots, M$, outside ϵ_ρ with residues Res $f(z_m)$. Then, performing the contour integral of (38) yields

$$V_k^N(f)=-\frac{2}{\pi}\sum_{m=1}^{M}\operatorname{Res} f(z_m)\frac{\tilde{U}_k(z_m)}{\omega_{N+1}(z_m)},\quad k\geqslant 0. \tag{50}$$

Defining

$$r=\min_{1\leqslant m\leqslant M}\left|z_m+\sqrt{z_m^2-1}\right|>1,$$

we can see from (50) that $\rho<r$ and $|V_k^N|=O(r^{-k-N})$. This fact and (41) permit us to estimate the error

$$|Q(K, f)-Q_N(K, f)|\leqslant\Omega(K)\sum_{k=0}^{\infty\,\prime}|V_k^N(f)|\lesssim\Omega(K)|V_0^N(f)|\frac{r+1}{2(r-1)}, \tag{51}$$

where $A\lesssim B$ indicates that $A\leqslant B'$ holds and that B is an approximation to B'.

Now, we wish to estimate $|V_0^N(f)|$ in terms of the available coefficients a_k^N of $p_N(t)$. Elliott [4] gives

$$a_k^N=\frac{2}{\pi i}\oint_{\epsilon_\rho}\frac{T_{N-k}(z)f(z)}{\omega_{N+1}(z)}\,\mathrm{d}z,\quad 0\leqslant k\leqslant N.$$

Performing the contour integral and comparing the result with (50) gives relations $|V_0^N| \sim |a_N^N| r/(r^2-1)$ and $|a_k^N| \sim r|a_{k+1}^N|$, unless the poles z_m are close to the range $[-1, 1]$ on the real axis. From these relations and (51), we have

$$|Q(K, f) - Q_N(K, f)| \lesssim \Omega(K)\left(\tfrac{1}{2}|a_N^N|\right)\frac{r}{(r-1)^2}. \tag{52}$$

The constant r may be estimated from the asymptotic behavior of $\{a_k^N\}$ [13].

Next, we wish to estimate the error (43) in terms of the computed B_k^σ, which is expressed in the contour integral [11]

$$B_k^\sigma = \frac{-1}{\pi i}\oint_{\epsilon_p} \frac{T_{N/\sigma-k}(z) f(z)\, dz}{\omega_{N+1}(z)\{T_{N/\sigma}(z) - \cos 2\pi\beta_\sigma\}}, \quad 1 \leqslant k \leqslant \frac{N}{\sigma}, \ \sigma = 2, 4, \tag{53}$$

where the right-hand side of (53) is multipled by $\frac{1}{2}$ when $k = N/\sigma$. Performing the contour integrals in (39) and (53) and comparing both results yield estimates $|V_0^{N+N/\sigma}| \sim 4|B_{N/\sigma}^\sigma| r/(r^2-1)$, $|V_k^{N+N/\sigma}| = O(r^{-k-N-N/\sigma})$ and $|B_k^\sigma| \sim r|B_{k+1}^\sigma|$. Using these relations and (44) in (43) yield estimates of the truncation errors for the approximates $Q_{N+N/\sigma}(K, f)$, $\sigma = 2, 4$, as follows:

$$|Q(K, f) - Q_{N+N/\sigma}(K, f)| \lesssim 2\Omega(K)(1 + |\cos 2\pi\beta_\sigma|)|B_{N/\sigma}^\sigma|\frac{r}{(r-1)^2}. \tag{54}$$

The relations (52) and (54) with (45)–(47) indicate that the errors can be estimated independently of the value of c.

5. Numerical examples

We show here numerical results by the present automatic quadrature scheme for the following definite integrals of algebraic singularity $|t-c|^\alpha$ with $\alpha = -0.7$, in particular:

(A) $\int_{-1}^{1} e^{a(t-1)}|t-c|^\alpha\, dt$, $\quad a = 4, 8, 16$, $\quad c = 0.2, 1.0$,

(B) $\int_{-1}^{1} (t^2+a^2)^{-1}|t-c|^\alpha\, dt$, $\quad a = 1, \frac{1}{4}, \frac{1}{8}$, $\quad c = 0.2, 1.0$,

(C) $\int_{0}^{1} \cos(2\pi a t)|t-c|^\alpha\, dt$, $\quad a = 8.1, 16.1, 32.1$, $\quad c = 0.5, 1.0$,

(D) $\int_{0}^{1} \frac{1-a^2}{1-2at+a^2}|t-c|^\alpha\, dt$, $\quad a = 0.8, 0.9, 0.95$, $\quad c = 0.6, 1.0$,

(E) $\int_{0}^{1} \sqrt{e^t - 1}\,|t-c|^\alpha\, dt$, $\quad c = 0.6, 1.0$.

There does not seem to exist any automatic quadrature rule to be compared for indefinite integrals of product type integration (1).

In Table 1 we compare the results of the present scheme with those of QAWS (and QAGP) in the subroutine package QUADPACK [16]. Table 1 lists the numbers of sample points required to satisfy the requested relative tolerances ϵ_r. In Table 1, only for reference, we list the results

Table 1
Comparison of the performances of the present method and QUADPACK

Problem	a	c	$\epsilon_r = 10^{-6}$		$\epsilon_r = 10^{-10}$	
			Present method	QUAD-PACK	Present method	QUAD-PACK
A	4	0.2	17	630 *	21	798 *
		1.0	⇓	40	⇓	40
	8	0.2	25	630 *	33	798 *
		1.0	⇓	40	⇓	80
	16	0.2	33	462 *	41	714 *
		1.0	⇓	40	⇓	120
B	1	0.2	21	630 *	33	798 *
		1.0	⇓	40	⇓	40
	$\frac{1}{4}$	0.2	81	630 *	129	882 *
		1.0	⇓	70	⇓	170
	$\frac{1}{8}$	0.2	161	714 *	257	966 *
		1.0	⇓	200	⇓	230
C	8.1	0.5	49	630 *	65	882 *
		1.0	⇓	240	⇓	490
	16.1	0.5	81	798 *	97	1218 *
		1.0	⇓	490	⇓	980
	32.1	0.5	161	1134 *	161	2058 *
		1.0	⇓	980	⇓	1950
D	0.8	0.6	65	672 *	97	1218 *
		1.0	⇓	120	⇓	200
	0.9	0.6	129	840 *	193	1050 *
		1.0	⇓	200	⇓	280
	0.95	0.6	257	1008 *	513	1470 *
		1.0	⇓	280	⇓	360
E [a]		0.6	65	462 *	1025	630 *
		1.0	⇓	70	⇓	220

[a] The numbers of abscissae in the third and fourth columns for the problem (E) are those for $\epsilon_r = 10^{-3}$, while those in the fifth and sixth columns are the numbers of abscissae for $\epsilon_r = 10^{-5}$.

with asterisks by QAGP, which can manage to give approximations to the integrals of interior singular kernels $K(t;\, c)$ not only algebraic but of any type without using any knowledge of the singularity except for the singular point. Therefore, the results by QAGP would not be favourably compared with those of the present method. It appears difficult to find any automatic quadrature program for integrals with interior point singularity other than QAGP.

We note that the present scheme can efficiently give all the approximations of the integrals (1) for a set of the values of c by using a common number of function evaluations once and for all for smooth functions.

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